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Valence 2084

Claims:

- 1. A lithium ion battery which comprises a positive electrode and a negative electrode; said positive electrode having an active material represented by the formula Li_aM'_(2-b)M"_bP₃O_{12-c}Z_c, 0 ≤ b ≤ 2, 0 < c < 12, a is greater than zero and selected to represent the number of Li atoms to balance said formula; where M' and M" are the same or different from one another and are each elements selected from the group consisting of metal and metalloid elements; and where Z is a halogen.</p>
 - 2. The battery of claim 1 wherein the halogen is F (fluorine).
 - 3. The battery of claim 1 wherein said active material is represented by the formula $\text{Li}_a\text{M'}_{(2-b)}\text{M"}_b\text{P}_3\text{O}_{12-c}\text{F}_c$; M' is selected from the group consisting of: V, Fe, Mn, and M" is selected from the group consisting of: V, Fe, Mn, Ti, Cr, Co, Ni, Cu, and Mo.
- 4. The battery of claim 1 wherein said active material is represented by one of the following formulas $\text{Li}_{2.0}\text{M'}_{(2-b)}\text{M''}_{b}\text{P}_{3}\text{O}_{11}\text{F};$ $\text{Li}_{2.5}\text{M'}_{(2-b)}\text{M''}_{b}\text{P}_{3}\text{O}_{11.5}\text{F}_{0.5};$ $\text{Li}_{3}\text{M'}_{(2-b)}\text{M''}_{b}\text{P}_{3}\text{O}_{11.5}\text{F}_{0.5};$ and $\text{Li}_{3}\text{M'}_{(2-b)}\text{M''}_{b}\text{P}_{3}\text{O}_{11}\text{F}.$
- 5. The battery of claim 1 wherein said positive electrode active material is selected from the group consisting of: $\text{Li}_{2.5}\text{V}^{3+}_{1.0}\text{V}^{3+}_{1.0}\text{P}_3\text{O}_{11.5}\text{F}_{0.5};$ $\text{Li}_{2.0}\text{V}^{3+}_{1.0}\text{V}^{3+}_{1.0}\text{P}_3\text{O}_{11.0}\text{F}_{1.0};$ $\text{Li}_{2.5}\text{V}^{3+}_{1.0}\text{Mn}^{3+}_{1.0}\text{P}_3\text{O}_{11.5}\text{F}_{0.5};$ $\text{Li}_{2.0}\text{V}^{3+}_{0.5}\text{Fe}^{3+}_{1.5}\text{P}_3\text{O}_{11.0}\text{F};$ $\text{Li}_3\text{V}^{2+}_{0.5}\text{V}^{3+}_{1.5}\text{P}_3\text{O}_{11.5}\text{F}_{0.5};$ $\text{Li}_3\text{V}^{2+}_{0.5}\text{V}^{3+}_{1.5}\text{P}_3\text{O}_{11.5}\text{F}_{0.5};$ $\text{Li}_3\text{V}^{2+}_{0.5}\text{V}^{3+}_{1.5}\text{P}_3\text{O}_{11.5}\text{F}_{0.5};$

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- 6. The battery of claim 1 wherein M' and M" are the same transition metal or are different transition metals.
- 7. The battery of claim 1 wherein at least one of M' and M" is selected from the group of transition metals.
- 8. The battery of claim 1 wherein M' and M''
 are metals or metalloids independently selected from the
 group consisting of: V, Fe, Mn, Ti, Cr, Co, Ni, Cu, Mo,
 Al, Mg, Ca, B, Zn, Sn.
 - 9. The battery of claim 1 wherein said positive electrode active material is represented by the formula $\text{Li}_3\text{M'}_{(2-b)}\text{M"}_b\text{P}_3\text{O}_{12-c}\text{F}_c$; M'and M" each have a valence state which is the same or different, where said valence state is +2 or +3.
- 20 10. The battery of claim 1 wherein said positive electrode active material is characterized by deintercalating lithium ions during charging cycle of said battery; said negative electrode active material characterized by intercalating said deintercalated lithium ions during said charging cycle, and by subsequent deintercalation of lithium ions during discharge cycle; and said positive electrode active material further characterized by reintercalating said discharge cycle lithium ions.
 - 11. An electrochemical cell having an electrode which comprises an active material represented by the following formula:
- 35 $\text{Li}^{+1}_{(a-x)}$ $\text{MII}^{d}_{(2-b)}$ MII^{e}_{b} P^{+5}_{3} O^{-2}_{12-c} Z^{-1}_{c} ;

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(A) where each superscript value represents the oxidation states of respective elements in a first condition, x = 0:

Superscript +1 is the oxidation state of one atom of Li (lithium),

Superscript d is the oxidation state of one atom of MI,

Superscript e is the oxidation state of one atom of MII,

Superscript -1 is the oxidation state of one atom of Z which is a halogen,

Superscript +5 is the oxidation state of one atom of P (phosphorus) and in the case of P_3 constitutes a total of 15,

Superscript -2 is the oxidation state of one atom of O (oxygen);

- (B) MI and MII are the same or different and are each elements independently selected from the group of metal and metalloid elements;
- (C) a, c, d and e are each greater than zero; d and e are each at least one; $0 \le b \le 2$; c is less than 12; and where a, b, c, d and e fulfill the requirement: $(a \times 1) + ((2 b) \times d) + (b \times e) + 15 = (1 \times c) + ((12 c) \times 2)$; and
 - (D) in a second condition represented by said formula with $0 < x \le a$, and in said second condition, said oxidation state of MI is represented by d' and said oxidation state of MII is represented by e', said amount X of Li is removed from said compound, accompanied by a change in oxidation state of at least one of said MI and MII, according to $((2-b) \times (d'-d)) + (b(e'-e)) = X$; where $d' \ge d$ and $e' \ge e$; and where d, d', e, and e' are each less than or equal to 8.

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- 12. The battery of claim 11 wherein the halogen is F (fluorine).
- 13. The cell according to claim 11 wherein d and e are each at least 2, $0 \le b \le 2$, and d, d', e, and e' are each less than or equal to 6.
 - 14. The cell according to claim 11 wherein d, d', e and e' are each less than or equal to 7; and at least one of the following two conditions are met: (1) d' > d and (2) e' > e.
 - 15. The cell according to claim 11 wherein MI and MII are each independently selected from the group consisting of: V, Fe, Mn, Ti, Cr, Co, Ni, Cu, Mo, Al, Mg, Ca, B, Zn, Sn.
 - 16. An electrode having an active material in a first condition represented by the formula $\text{Li}_{3-x}\text{E'}_{(2-b)}\text{E"}_b\text{P}_3\text{O}_{12-c}\text{F}_c$, x=0, $0 \le b \le 2$, 0 < c < 12; where at least one of E' and E" is an element selected from the group consisting of metals and metalloids; and E' and E" are the same or different from one another; and in a second condition by said formula where $0 < x \le 3$; and where at least one of E' and E" has an oxidation state higher than its oxidation state in said first condition.
- 17. An electrode which comprises an active material, represented by the nominal general formula 30 Li_aM'_(2-b)M"_bP₃O_{12-c)}Z_c, 0 ≤ b ≤ 2, 0 < c < 12, a is greater than zero and selected to represent the number of Li atoms to balance said formula; where M' and M" are each elements selected from the group consisting of metal and metalloid elements, and said M' and M" are the same or different from one another; and where Z is a halogen.

- 18. The electrode of claim 17 wherein at least one of M' and M" is selected from the group of transition metals, and Z is F (fluorine).
- 5 19. The electrode of claim 17 wherein M' and M" are each independently selected from the group consisting of transition metals, and Z is F (fluorine).
- 20. An electrode which comprises an active material, represented by the nominal general formula $\text{Li}_a\text{M'}_{(2-b)}\text{M"}_b\text{Si}_y\text{P}_{3-y}\text{O}_{12-c}\text{Z}_c$, $0 \le b \le 2$, 0 < c < 12, $0 \le y < 3$, a is greater than zero and selected to represent the number of Li atoms to balance said formula; where M' and M" are each elements selected from the group consisting of metal and metalloid elements, and said M' and M" are the same or different from one another; and where Z is a halogen.
 - 21. The electrode of claim 20 wherein at least one of M' and M" is selected from the group of transition metals, and Z is F (fluorine).
 - 22. The electrode of claim 20 where a is 3.